In Silico Design of Highly Selective Mo-V-Te-Nb-O Mixed Metal Oxide Catalysts for Ammoxidation and Oxidative Dehydrogenation of Propane and Ethane

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Computational details

The density functional calculations with periodic boundary conditions were performed using the Perdew-Burke-Ernzerhof (PBE) functional,[1] as implemented in the Quantum Espresso code. We used GBRV ultrasoft pseudopotentials[2] with a planewave basis set and a cutoff energy of 40 Ry for wavefunctions and 160 Ry for charge density. Electron smearing was employed using the Gaussian-smearing technique with a width of 0.01 Ry. All calculated values of energies have been extrapolated to $k_BT = 0$. All calculations were performed using the spin-polarized wavefunctions. For all surface calculations, only the gamma point is sampled because of the large model we used, and at least 15 Å vacuum spacing between adjacent images was used to prevent the interaction between the replicas along the *z*-direction.

The heat of formations for all the configurations were calculated using bulk V_2O_5,[3] Nb_2O_5,[4] α-TeO_2,[5] MoO_3,[6] and molecular O_2 as references. It should be noted that we only considered electronic energies and do not consider zero-point energy corrections, thermal corrections, and entropic corrections.

Figure S1. Atomic description of the active center (composed by two O=Te, one O=V(S2), two O=V(S4), two O=V(S7), and bridged oxygen atoms) in the configuration **3k**.

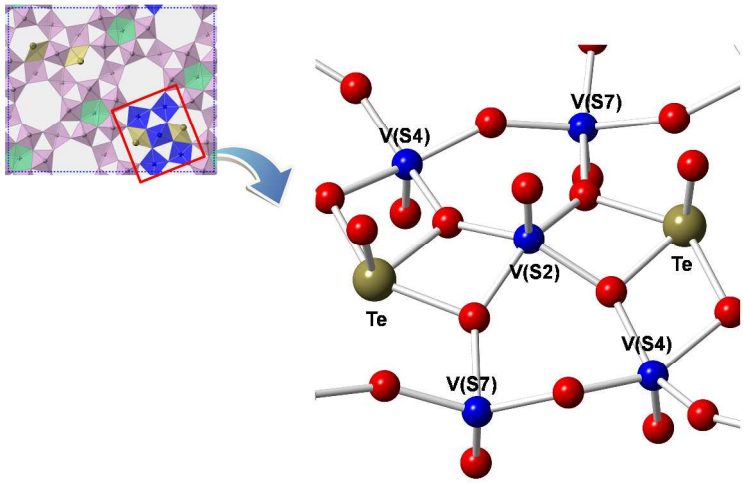

Table S1. The calculated electronic energies for all configurations studied in this work. The electronic energy for H is -1.000 Ry.

Species	Surface (Ry)	Surface-H (Ry)	D_{O-H} (kcal/mol)
0V Te(S12)O	-9338.763013	-9337.55149	66.4
0V Nb(S9)O	-9338.699504	-9337.55149	46.4
0V Mo(S11)O	-9338.67957	-9337.55149	40.2
0V_S2-S4-BridgeO	-9338.706986	-9337.55149	48.8
0V_S2-S7-BridgeO	-9338.698986	-9337.55149	46.3
0V_S4-S7-BridgeO	-9338.714409	-9337.55149	51.1
1V Te(S12)O	-9344.636585	-9343.424979	66.4
3a	-9350.472267	-9349.25987	66.6
3b	-9350.480892	-9349.268478	66.6
3c	-9350.490389	-9349.263728	71.1
3d	-9350.503634	-9349.266337	74.5
3e	-9356.333007	-9355.100506	72.9
3f	-9356.337935	-9355.098448	75.1
3g	-9356.333537	-9355.101321	72.9
3h	-9356.344867	-9355.105342	75.2
3i	-9362.176497	-9360.930732	77.1
3j	-9362.174297	-9360.93314	75.7
3k	-9368.005172	-9366.756554	78.0

References

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(5) Lindqvis.O *Acta Chem. Scand.* **1968**, *22*, 977.

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Cell parameters and atomic coordinates for the one-layer model (the 0V, 1V, and 5V (3k) cases).

a = 21.13438; b = 26.64700; c = 19.15640

Coordinates

(1) 0V

Mo	0.222422199	0.764789360	0.446042919
Mo	0.338656365	0.996407677	0.449426869
Mo	0.398958541	0.238993584	0.447636062
Mo	0.435543314	0.107414002	0.505946555
Mo	0.505111374	0.975979768	0.504010348
Mo	0.604863917	0.868844491	0.447339554
Mo	0.678671975	0.992354464	0.505962202

Mo	0.222829231	0.898283067	0.503103412
Mo	0.566375535	0.206640392	0.496007999
Mo	0.722380530	0.264795171	0.446043691
Mo	0.106182835	0.533134388	0.449497405
Mo	0.606178477	0.496428405	0.449413561
Mo	0.838655668	0.033141983	0.449498655
Mo	0.045785892	0.290588232	0.447729060
Mo	0.545843189	0.739002343	0.447643834
Mo	0.899021345	0.790586569	0.447713699
Mo	0.009212645	0.422172104	0.505992030
Mo	0.509256654	0.607416687	0.505923092
Mo	0.935593235	0.922166959	0.506023427
Mo	0.939729402	0.553627448	0.504013806
Mo	0.439715437	0.475979984	0.503959667
Mo	0.005104477	0.053629112	0.504041677
Mo	0.839990773	0.660768420	0.447328187
Mo	0.339960728	0.368844022	0.447318841
Mo	0.104838266	0.160775785	0.447350967
Mo	0.766132708	0.537272149	0.505930347
Mo	0.266167299	0.492338325	0.505938369
Mo	0.178704238	0.037263995	0.505943755
Mo	0.221975326	0.631301216	0.503100335
Mo	0.721996911	0.398296452	0.503064974
Mo	0.722856016	0.131308384	0.503101080
Mo	0.878367158	0.322997374	0.495971116

Mo	0.378426261	0.706637467	0.496003617
Mo	0.066432498	0.822978112	0.496000352
Nb	0.582050237	0.083239802	0.451884999
Nb	0.862771618	0.446418310	0.451810061
Nb	0.362760185	0.583233420	0.451865917
Nb	0.082047428	0.946404391	0.451851543
Te	0.768421822	0.879926467	0.477963835
Te	0.676412647	0.649667070	0.477890903
Te	0.176387131	0.379901604	0.477923595
Te	0.268397815	0.149652072	0.477902789
Mo	0.222417387	0.264793439	0.502212499
Mo	0.722426911	0.764790552	0.502206332
O	0.222414007	0.764790410	0.358795380
O	0.222443742	0.264794668	0.589325278
O	0.338110127	0.995473106	0.362046714
O	0.399257418	0.236702570	0.360426769
O	0.435451601	0.107071616	0.593607159
O	0.506333801	0.976336009	0.591588576
O	0.602806157	0.871832494	0.360131894
O	0.676674819	0.991291113	0.593467982
O	0.582263088	0.083204488	0.362538470
O	0.223364026	0.897281361	0.590736578
O	0.567112648	0.209579666	0.583507249
O	0.775071171	0.887292919	0.572957720
O	0.741946961	0.196556945	0.475921124

O	0.795046458	0.095923046	0.476762404
O	0.261661308	0.030313929	0.477729101
O	0.801612583	0.800592706	0.471013207
O	0.921054479	0.060446063	0.477428233
O	0.996933278	0.977971167	0.482909784
O	0.897194621	0.861434374	0.478055781
O	0.186920410	0.199206195	0.470211601
O	0.038919795	0.116402934	0.479203825
O	0.018108286	0.889321715	0.476940696
O	0.990357341	0.790699260	0.470815718
O	0.090873704	0.025361415	0.473056125
O	0.130493557	0.880271593	0.477187023
O	0.131565438	0.781237346	0.467477734
O	0.061858787	0.221796319	0.468578951
O	0.170078452	0.106555438	0.473508989
O	0.172797324	0.962801763	0.482908783
O	0.374962382	0.063001967	0.475374890
O	0.722374044	0.264788539	0.358802739
O	0.722421362	0.764770059	0.589329197
O	0.106741012	0.534000532	0.362121688
O	0.606743824	0.495503525	0.362039315
O	0.838112449	0.034010389	0.362117629
O	0.045457312	0.292867162	0.360521842
O	0.545552331	0.736718925	0.360427224
O	0.899354584	0.792874656	0.360497101

O	0.009211533	0.422514885	0.593646717
O	0.509339178	0.607059374	0.593583479
O	0.935581164	0.922502485	0.593690723
O	0.938488351	0.553239068	0.591585391
O	0.438472250	0.476333672	0.591530174
O	0.006340034	0.053253109	0.591618717
O	0.842089281	0.657803999	0.360123117
O	0.342013292	0.371825392	0.360119568
O	0.102744411	0.157813899	0.360149223
O	0.768076291	0.538351809	0.593430027
O	0.268188267	0.491261310	0.593436520
O	0.176789599	0.038344338	0.593448667
O	0.862582977	0.446520827	0.362463941
O	0.362521935	0.583198395	0.362517352
O	0.082224224	0.946506432	0.362504052
O	0.221346927	0.632307177	0.590727221
O	0.721464004	0.397299611	0.590687548
O	0.723484282	0.132312621	0.590727401
O	0.877562964	0.320134449	0.583470968
O	0.377678561	0.709573474	0.583506949
O	0.067219677	0.820106387	0.583510760
O	0.669752686	0.642254286	0.572884619
O	0.169751657	0.387295493	0.572928384
O	0.275076593	0.142260285	0.572901103
O	0.702855784	0.333041689	0.475935218

O	0.202867050	0.696547544	0.475922297
O	0.241957031	0.833031202	0.475948792
O	0.649781248	0.433681392	0.476796347
O	0.149787351	0.595908039	0.476771059
O	0.295047777	0.933663168	0.476825915
O	0.183170506	0.499264902	0.477871998
O	0.683164042	0.530322991	0.477756928
O	0.761660754	0.999274337	0.477853416
O	0.643237489	0.728987308	0.470988586
O	0.143210945	0.300597636	0.471025426
O	0.301584825	0.228988724	0.470988052
O	0.523767662	0.469157754	0.477358923
O	0.023781830	0.560437106	0.477414072
O	0.421065750	0.969143387	0.477384645
O	0.447877645	0.551642130	0.482859248
O	0.947888078	0.477976228	0.482855517
O	0.496933591	0.051642228	0.482900204
O	0.547652605	0.668151683	0.477953420
O	0.047617482	0.361435464	0.478048383
O	0.397150130	0.168143225	0.477952906
O	0.257875928	0.330397000	0.470191981
O	0.757900861	0.699200106	0.470177883
O	0.686941433	0.830390446	0.470210365
O	0.405900672	0.413204354	0.479130173
O	0.905913885	0.616402490	0.479188890

O	0.538931888	0.913206684	0.479170663
O	0.426721689	0.640291839	0.476952104
O	0.926698908	0.389333232	0.476901133
O	0.518079923	0.140292119	0.476975232
O	0.454497428	0.738890294	0.470726526
O	0.954452748	0.290713416	0.470815892
O	0.490304905	0.238887503	0.470725944
O	0.353957604	0.504254138	0.472956145
O	0.853957394	0.525364638	0.473032042
O	0.590866804	0.004260678	0.472995740
O	0.314338642	0.649331774	0.477325310
O	0.814319563	0.380287840	0.477135328
O	0.630473868	0.149339942	0.477336938
O	0.313270246	0.748348143	0.467458632
O	0.813234488	0.281255581	0.467451900
O	0.631531981	0.248355620	0.467471286
O	0.382910699	0.307797584	0.468487541
O	0.882958342	0.721790864	0.468555924
O	0.561898051	0.807800491	0.468511634
O	0.274753035	0.423052059	0.473517366
O	0.774758969	0.606551292	0.473485616
O	0.670087634	0.923051984	0.473544671
O	0.272029283	0.566799444	0.482914707
O	0.772030887	0.462815840	0.482874580
O	0.672800610	0.066810745	0.482908665

O	0.069850716	0.466570540	0.475515145
O	0.569845410	0.563008774	0.475355302
O	0.874967508	0.966568236	0.475530363

(2) 1V (at the S2 site)

Mo	0.222432894	0.764798708	0.446669505
Mo	0.338860617	0.996279511	0.449448736
Mo	0.399019133	0.238967226	0.447684318
Mo	0.435576228	0.107187414	0.505816479
Mo	0.505368808	0.975636737	0.503566804
Mo	0.606549334	0.868767585	0.448247444
Mo	0.679253385	0.991790802	0.505246818
Mo	0.222878167	0.898381197	0.503116281
Mo	0.566264586	0.206619490	0.496320163
Mo	0.722376252	0.264791852	0.446656903
Mo	0.105991286	0.533260724	0.449505942
Mo	0.605444731	0.495752472	0.449560049
Mo	0.839390483	0.033826947	0.449656014
Mo	0.045727687	0.290604676	0.447770621
Mo	0.545883126	0.739415471	0.448076656
Mo	0.898959657	0.790191253	0.448097002
Mo	0.009188446	0.422395809	0.505841713
Mo	0.509262382	0.606999523	0.505679420
Mo	0.935580909	0.922594091	0.505798676
Mo	0.939471679	0.553972991	0.503540119

Mo	0.439316806	0.475966976	0.503765338
Mo	0.005510764	0.053647131	0.503841505
Mo	0.838283685	0.660846504	0.448235866
Mo	0.339639681	0.368836427	0.447433142
Mo	0.105175178	0.160771423	0.447465056
Mo	0.765556537	0.537824515	0.505178519
Mo	0.265938256	0.492229316	0.505842598
Mo	0.178940371	0.037371701	0.505846064
Mo	0.221922929	0.631212001	0.503104478
Mo	0.722351081	0.398487758	0.503007361
Mo	0.722494128	0.131109639	0.503054912
Mo	0.878481011	0.323003528	0.496282481
Mo	0.378376251	0.706427225	0.496589357
Mo	0.066472781	0.823195205	0.496571683
Nb	0.581957388	0.083316721	0.451814973
Nb	0.862867734	0.446326167	0.451720290
Nb	0.362588815	0.583210318	0.451596728
Nb	0.082217583	0.946431022	0.451606649
Te	0.771981105	0.874832820	0.478625471
Te	0.672861354	0.654765100	0.478574297
Te	0.175455353	0.379623762	0.477945027
Te	0.269344317	0.149941222	0.477936833
Mo	0.222412692	0.264794916	0.502306085
V	0.722414537	0.764803866	0.499929770
O	0.222430305	0.764792965	0.359435806

O	0.222427348	0.264797533	0.589429993
O	0.338251231	0.995461177	0.362091776
O	0.399572864	0.236730275	0.360481935
O	0.435643606	0.106707884	0.593466557
O	0.506423387	0.976450969	0.591128936
O	0.604503322	0.872115559	0.361059877
O	0.677340294	0.991846001	0.592863392
O	0.582176475	0.083522641	0.362505255
O	0.223313589	0.897536095	0.590735127
O	0.566998272	0.209559858	0.583784108
O	0.777135295	0.887136534	0.572791819
O	0.741763897	0.196524890	0.476073739
O	0.794841635	0.095795742	0.476336424
O	0.261811740	0.030356646	0.477937030
O	0.803598481	0.799599642	0.471350931
O	0.921397763	0.061020573	0.477321428
O	0.997064364	0.978228375	0.481901326
O	0.896493079	0.862280627	0.476738664
O	0.187441170	0.199114559	0.470127824
O	0.039267483	0.116625406	0.479108625
O	0.018142220	0.889470751	0.477101294
O	0.990233777	0.791017159	0.472165829
O	0.091181293	0.025373883	0.472862684
O	0.130688059	0.880361740	0.477046145
O	0.131662415	0.781321779	0.467933681

O	0.062220524	0.221776670	0.468725114
O	0.169978274	0.106481067	0.473695497
O	0.172956897	0.962901942	0.482782911
O	0.374840424	0.062810108	0.475540026
O	0.722375634	0.264778978	0.359423363
O	0.722433629	0.764788464	0.582364363
O	0.106618261	0.534015190	0.362145590
O	0.605299567	0.495524821	0.362212365
O	0.839562552	0.033991536	0.362312790
O	0.045147945	0.292834782	0.360568118
O	0.544675550	0.737338792	0.360849477
O	0.900188130	0.792276339	0.360875079
O	0.009036955	0.422879654	0.593496085
O	0.508749033	0.606906134	0.593314142
O	0.936149412	0.922645302	0.593428192
O	0.938401902	0.553137474	0.591105467
O	0.438214010	0.476690458	0.591302693
O	0.006617211	0.052922144	0.591373561
O	0.840330458	0.657502338	0.361047951
O	0.341757449	0.371954167	0.360229044
O	0.103030506	0.157658314	0.360263636
O	0.767432380	0.537768626	0.592799244
O	0.268094337	0.491348205	0.593361526
O	0.176891620	0.038251943	0.593360492
O	0.862689222	0.446183347	0.362410490

O	0.362191289	0.583275033	0.362275160
O	0.082551538	0.946422703	0.362287317
O	0.221411809	0.632058311	0.590725999
O	0.721609618	0.397827242	0.590594822
O	0.723333370	0.131790019	0.590636862
O	0.877697692	0.320136817	0.583752658
O	0.377249654	0.708978392	0.584096347
O	0.067625956	0.820676733	0.584075890
O	0.667698623	0.642420859	0.572731696
O	0.169473309	0.387194265	0.572971026
O	0.275362350	0.142355738	0.572958953
O	0.703027581	0.333069208	0.476072471
O	0.202770766	0.696561145	0.476152083
O	0.242063979	0.833033672	0.476177321
O	0.649983889	0.433803867	0.476352853
O	0.149709309	0.595897001	0.476703341
O	0.295120834	0.933682485	0.476761544
O	0.183024265	0.499212260	0.478065606
O	0.683038372	0.530718547	0.477625385
O	0.761786504	0.998887960	0.477747763
O	0.641234431	0.730002418	0.471360457
O	0.143005678	0.300495254	0.471105939
O	0.301787827	0.229079548	0.471078299
O	0.523425626	0.468582527	0.477237879
O	0.023666019	0.560731475	0.477252911

O	0.421183287	0.968850202	0.477249289
O	0.447751301	0.551387951	0.481817608
O	0.948269091	0.477977451	0.481800246
O	0.496552006	0.051634802	0.481842599
O	0.548340893	0.667322070	0.476657708
O	0.048121918	0.361661719	0.477792494
O	0.396645568	0.167910493	0.477709951
O	0.257366261	0.330476576	0.470102280
O	0.756783303	0.698835239	0.470154099
O	0.688051394	0.830774368	0.470158281
O	0.405555080	0.412982490	0.479051883
O	0.906051737	0.616539745	0.479095849
O	0.538784262	0.913069289	0.479106321
O	0.426686980	0.640153549	0.477086285
O	0.926846075	0.389205281	0.477169473
O	0.517940035	0.140405945	0.477255385
O	0.454607044	0.738592810	0.472132919
O	0.954647445	0.290781876	0.471083726
O	0.490107176	0.238803163	0.471008652
O	0.353654352	0.504239404	0.472752274
O	0.854063292	0.524522927	0.473633225
O	0.590762904	0.005102488	0.473650570
O	0.314138777	0.649251038	0.477160125
O	0.814475024	0.380220971	0.477534165
O	0.630318913	0.149391851	0.477735255

O	0.313185846	0.748286659	0.467924528
O	0.813214032	0.281166684	0.467906988
O	0.631548688	0.248431494	0.467914133
O	0.382556769	0.307804286	0.468658596
O	0.882252259	0.721658863	0.468513425
O	0.562591476	0.807947704	0.468525229
O	0.274850577	0.423114035	0.473687849
O	0.778420094	0.604800741	0.475100447
O	0.666397819	0.924810154	0.475161586
O	0.271868634	0.566701670	0.482787166
O	0.771703289	0.462933948	0.481856165
O	0.673121507	0.066682546	0.481939378
O	0.069980893	0.466749888	0.475641638
O	0.569537337	0.562013299	0.476517460
O	0.875281006	0.967585056	0.476722608

(3) 5V

Mo	0.222425434	0.764775474	0.444667207
Mo	0.337827151	0.995651759	0.449882474
Mo	0.398908521	0.238263117	0.447528378
Mo	0.435342189	0.106239717	0.505396112
Mo	0.504988460	0.973115057	0.501526913
V	0.603990731	0.865217904	0.452866717
Mo	0.678414143	0.988704687	0.503425325
Mo	0.221260223	0.897756585	0.503169850

Mo	0.566165710	0.206033865	0.496256232
Mo	0.722412264	0.264779267	0.447385258
Mo	0.107001848	0.533946420	0.449963834
Mo	0.606204599	0.496581149	0.448871611
Mo	0.838655783	0.033000731	0.449085291
Mo	0.045847573	0.291336422	0.447566792
V	0.546268033	0.743229280	0.451486082
V	0.898533770	0.786382316	0.451487923
Mo	0.009436725	0.423386127	0.505446239
Mo	0.511806760	0.610150022	0.502690778
Mo	0.933037737	0.919402564	0.502859719
Mo	0.939840105	0.556525257	0.501524709
Mo	0.440340253	0.477429403	0.503832810
Mo	0.004506964	0.052135580	0.504087710
V	0.840802179	0.664383681	0.452777075
Mo	0.341567746	0.369095586	0.448373058
Mo	0.103187311	0.160488768	0.448501220
Mo	0.766400337	0.540914601	0.503355913
Mo	0.267099081	0.492549831	0.506402655
Mo	0.177793473	0.037042258	0.506564952
Mo	0.223628289	0.631795957	0.503176293
Mo	0.723354794	0.399432559	0.501986122
Mo	0.721491916	0.130168353	0.502141264
Mo	0.878602887	0.323634717	0.496177295
Mo	0.380062711	0.708105832	0.494232920

Mo	0.064773039	0.821446809	0.494275183
Nb	0.581453072	0.082247879	0.451947453
Nb	0.863392151	0.447422231	0.451821582
Nb	0.363897411	0.583791875	0.451717171
Nb	0.080964912	0.945804315	0.451914214
Te	0.770098198	0.871595487	0.476763298
Te	0.674665878	0.658017274	0.476701950
Te	0.177036026	0.379943041	0.477841342
Te	0.267682518	0.149636071	0.477835862
Mo	0.222395294	0.264802698	0.501448765
V	0.722404993	0.764791014	0.500750126
O	0.222411584	0.764749983	0.357456893
O	0.222414491	0.264827160	0.588538166
O	0.335918653	0.995282361	0.362582833
O	0.399438752	0.236150932	0.360337875
O	0.435116652	0.105906156	0.593031336
O	0.504856998	0.974100813	0.589224597
O	0.603495682	0.866601286	0.370406898
O	0.676882577	0.989286952	0.591201531
O	0.581466434	0.082803323	0.362644843
O	0.221858908	0.895847954	0.590724648
O	0.566256251	0.209086714	0.583699364
O	0.777854050	0.888971605	0.569237856
O	0.740996198	0.196051358	0.475507035
O	0.793746180	0.094315312	0.474995752

O	0.260575536	0.029734158	0.479551466
O	0.801630331	0.797442163	0.473814021
O	0.920140855	0.059389150	0.476901530
O	0.995894590	0.977217293	0.481938781
O	0.895708955	0.860035159	0.475144849
O	0.186312098	0.199142551	0.469966340
O	0.038058680	0.116077141	0.479963231
O	0.016956545	0.888274952	0.475548232
O	0.989603189	0.790583194	0.470846972
O	0.090348457	0.025319344	0.473083665
O	0.129722530	0.880023603	0.476487193
O	0.130837792	0.780726157	0.465016419
O	0.061294506	0.222085750	0.468861556
O	0.169168261	0.106387177	0.474293088
O	0.171415745	0.962699105	0.484644578
O	0.374309398	0.061762522	0.475880523
O	0.722398545	0.264738439	0.360159062
O	0.722422022	0.764753348	0.583150660
O	0.108865660	0.534295174	0.362665653
O	0.605513186	0.496187167	0.361540105
O	0.839375892	0.033412517	0.361752569
O	0.045329291	0.293447424	0.360377664
O	0.547654458	0.742939433	0.369086046
O	0.897147913	0.786727241	0.369088435
O	0.009556039	0.423682592	0.593080655

O	0.511468259	0.610135468	0.590428314
O	0.933358025	0.919345126	0.590602177
O	0.939913429	0.555565656	0.589219054
O	0.439589429	0.477720797	0.591304745
O	0.005250207	0.051861087	0.591561880
O	0.841270433	0.663005798	0.370322070
O	0.343665367	0.372422848	0.361206576
O	0.101067216	0.157113093	0.361338516
O	0.767877507	0.540307895	0.591129082
O	0.269704815	0.491116582	0.593895957
O	0.175320371	0.038534275	0.594059134
O	0.863436200	0.446925441	0.362521556
O	0.362644931	0.582939438	0.362437725
O	0.082207746	0.946743133	0.362633461
O	0.223130696	0.633641734	0.590731707
O	0.721773754	0.398703938	0.589515639
O	0.723097083	0.130930900	0.589671419
O	0.878439066	0.320681652	0.583626596
O	0.377696599	0.711093511	0.581821538
O	0.067142572	0.818421995	0.581864012
O	0.666936247	0.640627391	0.569152384
O	0.170522223	0.387149620	0.572831505
O	0.274284166	0.142454663	0.572842230
O	0.703842833	0.333537217	0.475412409
O	0.203936985	0.696793080	0.474789613

O	0.240920600	0.832773536	0.474699948
O	0.651106054	0.435269502	0.474802477
O	0.151243467	0.596149664	0.477515228
O	0.293604328	0.933428113	0.477447113
O	0.184278690	0.499843210	0.479554656
O	0.683941819	0.532490720	0.475626180
O	0.760894967	0.997110252	0.475778463
O	0.643154338	0.732175148	0.473804309
O	0.143361167	0.300798274	0.470367075
O	0.301394318	0.228794999	0.470329618
O	0.524706145	0.470172965	0.476643408
O	0.024304815	0.562120522	0.475527897
O	0.420537740	0.967517334	0.475462509
O	0.448961929	0.552353674	0.481700234
O	0.948972782	0.478845386	0.481278261
O	0.495857068	0.050801333	0.481285536
O	0.549134131	0.669543293	0.475044702
O	0.048518893	0.362371219	0.477219705
O	0.396278642	0.167248959	0.477187442
O	0.258432787	0.330458795	0.469899922
O	0.758445098	0.700843187	0.473914638
O	0.686336776	0.828767199	0.474013976
O	0.406749622	0.413500338	0.479741678
O	0.906097269	0.617594623	0.477892148
O	0.538726753	0.912025079	0.477986237

O	0.427897118	0.641302521	0.475420119
O	0.927130398	0.389875735	0.477551910
O	0.517679294	0.139780080	0.477655245
O	0.455222523	0.738999687	0.470821846
O	0.954814501	0.291603151	0.470654665
O	0.489957285	0.238030100	0.470629029
O	0.354510386	0.504267090	0.472786185
O	0.854826162	0.525641447	0.473429524
O	0.590003892	0.004000177	0.473464980
O	0.315135878	0.649545203	0.476427575
O	0.815023700	0.380697208	0.477174336
O	0.629784746	0.148936694	0.477456866
O	0.314002249	0.748839750	0.465003707
O	0.813209279	0.281363272	0.468498688
O	0.631601516	0.248247264	0.468544645
O	0.383437545	0.307504959	0.468824281
O	0.882472926	0.721951972	0.476036601
O	0.562316425	0.807648901	0.476106446
O	0.275658573	0.423205987	0.474186682
O	0.780444300	0.606085629	0.475662331
O	0.664373975	0.923538508	0.475703201
O	0.273434992	0.566878235	0.484402508
O	0.772260759	0.463802723	0.481431906
O	0.672580704	0.065829661	0.481534664
O	0.070516302	0.467863015	0.476058864

O	0.570758937	0.563763100	0.474135630
O	0.874086204	0.965810068	0.474348312